

10/607,220

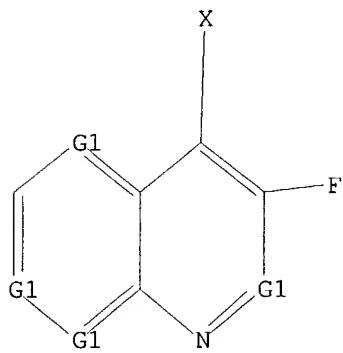
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L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS
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Structure attributes must be viewed using STN Express query preparation.

=> s 11 full
L3 39 SEA SSS FUL L1

=> file ca

=> s 13
L4 40 L3

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=> s 13/prep
        40 L3
        3150725 PREP/RL
L5      22 L3/PREP
        (L3 (L) PREP/RL)
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=> d ibib abs fhitstr 1-22

L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:247717 CA
 TITLE: Preparation of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor
 INVENTOR(S): Scarborough, Robert M.; Pandey, Anjali
 PATENT ASSIGNEE(S): Millennium Pharmaceuticals, Inc., USA
 SOURCE: PCT Int. Appl., 151 pp.
 CODEN: PIIXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072578	A2	20020919	WO 2002-US7187	20020308
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MN, MM, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	US 2003004158	A1 20030102	US 2002-94191 20020308	
PRIORITY APPN. INFO.:			US 2001-273951P	P 20010308
OTHER SOURCE(S):	MARPAT 137:247717			

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; V = O, S, N(CN); W = (un)substituted 1,4-piperazinediyl, 1,4-homopiperazinediyl; X = H, TZ, F, Cl; Z = OH, CN, CHO; T = c1-16 alkylidene optionally interrupted by O, S, CO2, OCO, CO; R1

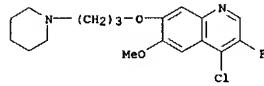
= H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R2 = H, (un)substituted C1-16 alkyl, C2-16 alkenyl, etc.; R3-R6 = H, halo, alkyl, etc.] which inhibit phosphorylation of the PDGF receptor to hinder abnormal cell growth and cell wandering, and a method for preventing or treating cell-proliferative diseases such as arteriosclerosis, vascular reobstruction, cancer and glomerulosclerosis, were prep'd. Thus, reacting 4-chloro-6-methoxy-7-(3-piperidylpropoxy)quinoline-3-carbonitrile (prepn. given with N-(4-isopropoxyphenyl)piperazinecarboxamide hydrochloride in the presence of K2CO3 in DMF afforded 69% II which showed IC50 of 0.134 .mu.M and 0.060 .mu.M in MG63 w/human plasma phosphorylation assay and in HR5 phosphorylation assay, resp.

IT 460088-42-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. of 4-piperazinoquinolines which inhibit phosphorylation of a PDGF receptor)

RN 460088-42-0 CA

L5 ANSWER 1 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 CN Quinoline, 4-chloro-3-fluoro-6-methoxy-7-[3-(1-piperidinyl)propoxy]- (9CI)
 (CA INDEX NAME)



L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 136:386033 CA

TITLE: Heterocyclylalkyl piperidine derivatives, particularly

INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Yousssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel;

PATENT ASSIGNEE(S): Viviani, Fabrice
 Aventis Pharma S.A., Fr.
 SOURCE: PCT Int. Appl., 362 pp.

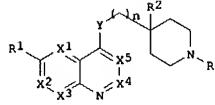
DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

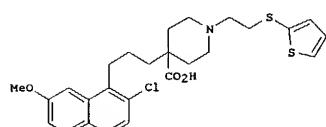
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	FR 2816618	AI 20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR	BR 2001015312	A	20030923	BR 2001-15312 20011114
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514
PRIORITY APPN. INFO.:			FR 2000-14738	A 20001115
			US 2000-255145P	P 20001214
OTHER SOURCE(S):	MARPAT 136:386033			

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L5 ANSWER 2 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



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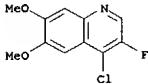


II

AB The invention concerns heterocyclylalkyl piperidine derivs. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO2H, alkoxy carbonyl, (un)substituted NH2, etc.; R2 = CO2H, alkoxy carbonyl, cycloalkyl carbonyl, cyano, CONR4R5, CH2OH, substituted alkyl, CF2-Rc, C(CH3)2-Rc, CR, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; R3, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NR4R5 = (un)substituted 5- or 6-membered heterocycle; Rc = CO2H, alkoxy carbonyl, cycloalkyl carbonyl, CONR4R5; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), C(F)2, C(=NOH), alkoxy iminomethylene, cycloalkyl oxy iminomethylene, or cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO2H, alkoxy carbonyl, NR4R5, CONR4R5; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prep'd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (preps. of both compds. given), followed by removal of the BOC group with CF3CO2H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis

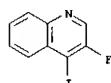
of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I are active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with *Staphylococcus aureus* IPB203 at 18-150 mg/kg s.c., or 40 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).
 IT 213772-63-5P, 3-Fluoro-4-iodoquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP

L5 ANSWER 4 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 reaction of 4-chloro-6,7-dimethoxy-3-fluoroquinoline (prepn. given) and
 4-(2-methoxyphenoxy)aniline gave
 4-(2-methoxyphenoxy)anilino-3-fluoro-6,7-
 dimethoxyquinoline.
 IT RL: RCT (Reactant); SPN (Synthetic preparation); PRMP
 (Preparation); RACT (Reactant or reagent)
 (prepn. of quinoline derivs. as inhibitors of MEK enzymes)
 RN 205448-48-2 CA
 CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)



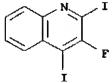
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 5 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 132:3495 CA
 TITLE: First total synthesis of cryptomisrine
 AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis;
 Godard, Alain; Queguiner, Guy
 CORPORATE SOURCE: UPRES-A 6014 - IRCOF/INSA de Rouen, Mont Saint Aignan,
 SOURCE: 76131, Fr.
 PUBLISHER: Tetrahedron (1999), 55(41), 12149-12156
 DOCUMENT TYPE: Elsevier Science Ltd.
 LANGUAGE: Journal
 OTHER SOURCE(S): English
 AB The first total synthesis of cryptomisrine, a novel
 indolo[3,2-b]quinoline
 dimeric alkaloid from Cryptolepis sanguinolenta, is reported. The approach is based on a convergent methodol. which involves a new halogen-dance reaction in 3-fluoro-4-iodoquinoline followed by its cross-coupling reaction to give bis-2-iodo-3-fluoroquinolin-4-ylmethanol which couples with 2-pivalaylaminophenylboronic acid and then heterocyclizes to cryptomisrine.
 IT 213772-63-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PRMP
 (Preparation); RACT (Reactant or reagent)
 (total synthesis of cryptomisrine)
 RN 213772-63-5 CA
 CN Quinoline, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 6 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 129:276078 CA
 TITLE: First halogen-dance reaction in quinoline series: application to a new synthesis of quindoline
 AUTHOR(S): Arzel, Erwan; Rocca, Patrick; Marsais, Francis;
 Godard, Alain; Queguiner, Guy
 CORPORATE SOURCE: UPRESA 6014 CNRS - IRCOF/INSA de Rouen, Mont Saint Aignan, 76131, Fr.
 SOURCE: Tetrahedron Letters (1998), 39(36), 6465-6466
 CODEN: TELEAY; ISSN: 0040-4039
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREFACT 129:276078
 AB The first halogen-dance reaction in the quinoline series is described and was applied to a new convergent synthesis of quindoline, a natural benzo-.delta.-carboline.
 IT 213772-72-6P
 RL: SPN (Synthetic preparation); PRMP (Preparation)
 (halogen-dance reaction in quinolines)
 RN 213772-72-6 CA
 CN Quinoline, 3-fluoro-2,4-diiodo- (9CI) (CA INDEX NAME)

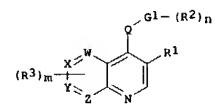


REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

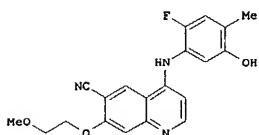
L5 ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 128:270546 CA
 TITLE: Quinoline derivatives inhibiting the effect of growth factors such as VEGF
 INVENTOR(S): Thomas, Andrew Peter; Hennequin, Laurent Francois Andre; Ple, Patrick Alan
 PATENT ASSIGNEE(S): Zeneca Ltd., UK; Zeneca Pharma S.A.; Thomas, Andrew Peter; Hennequin, Laurent Francois Andre; Ple, Patrick
 SOURCE: PCT Int. Appl., 129 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9813350	A1	19980402	WO 1997-GB2587	19970923
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, N2, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TT, RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BU, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG	AU 9743137	19980417	AU 1997-43137	19970923
AU 9743137	A1	19980417	AU 1997-43137	19970923
AU 733551	B2	20010517		
EP 929526	A1	19990721	EP 1997-941115	19970923
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI	CN 1237963	A	CN 1997-199929	19970923
CN 1237963	A	19991208	JP 1998-515386	19970923
JP 2001506890	T2	20010123	JP 1998-515386	19970923
NO 9901423	A	19990511	NO 1999-1423	19990324
KR 2000048575	A	20000725	KR 1999-702502	19990324
PRIORITY APPLN. INFO.: EP 1996-402034	A		EP 1996-402034	19960925
OTHER SOURCE(S): MARPAT 128:270546			WO 1997-GB2587	W 19970923
GI				

LS ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



I



II

AB The invention relates to the use of compds. I [R1 = F or H; R2 = OH, halo, Cl-3 alkyl, Cl-3 alkoxy, Cl-3 alkanoyloxy, CF3, cyano, amino, or NO2; n = 0-5; Q = O, NH, S, or CH2; G1 = Ph or 5- to 10-membered heteroarom. cyclic or bicyclic contg. O, S, and/or N; W, X, Y, Z = CH or N (but all 4 noted); N; m = 1-3; R3 = H, OH, halo, cyano, NO2, CF3, Cl-3 alkyl, NR4R5 (wherein R4 and R5 = H or Cl-3 alkyl), or R6X1- wherein X1 = CH2 or heteroatom linker group, and R6 = alkyl, alkenyl or alkynyl chain (un)substituted by OH, amino, NO2, alkyl, cycloalkyl, alkoxyalkyl, (un)substituted pyridone, Ph, heterocyclyl, etc. (which alkyl, alkenyl or alkynyl chain may have heteroatom linker), and salts thereof, in the manuf. of medicaments for prodn. of an antiangiogenic and/or vascular permeability-reducing effect. Also disclosed are processes for the prepn. of I, and pharmaceutical compns. contg. them as active ingredients. I and salts inhibit the effects of VEGF, a property useful in the treatment of a no. of disease states including cancer and rheumatoid arthritis (no data). Examples include 63 syntheses and 7 general formulations. For instance, condensation of 4-chloro-6-cyano-7-(2-methoxyethoxy)quinolone hydrochloride with 2-fluoro-5-hydroxy-4-methylaniline (preps. given) in refluxing iso-PROH gave 68% title compd. II, isolated as the HCl salt.

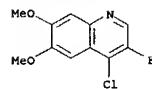
IT 205448-48-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of quinoline derivs. as growth factor inhibitors)

RN 205448-48-2 CA

CN Quinoline, 4-chloro-3-fluoro-6,7-dimethoxy- (9CI) (CA INDEX NAME)

LS ANSWER 7 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: THIS

17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

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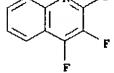
LS ANSWER 8 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 127:346280 CA
TITLE: Reactions of trifluorovinylolithium and 1-chloro-2,2-difluorovinylolithium: the synthesis of fluorinated heterocycles
AUTHOR(S): Burdon, J.; Coe, P. L.; Haslock, I. B.; Powell, R. L.
CORPORATE SOURCE: School of Chemistry, The University, Edgbaston, Birmingham, B15 2TT, UK
SOURCE: Journal of Fluorine Chemistry (1997), 85(2), 151-153
CODEN: JFLCAR; ISSN: 0022-1139
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Trifluorovinylolithium (from 1,1,2-tetrafluoroethane [HCFC-134a]) reacted with 2-trifluoromethylaniline at -78°C to give 2,3,4-trifluoroquinoline in moderate to good yield. In a similar reaction, 1-chlorodifluorovinylolithium (from 1-chloro-2,2-difluoroethane [HCFC-133a]) yielded 3-chloro-2,4-difluoroquinoline.

IT 198128-72-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of fluorinated heterocycles)

RN 198128-72-2 CA

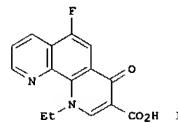
CN Quinoline, 2,3,4-trifluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

LS ANSWER 9 OF 22 CA COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 122:133124 CA
TITLE: Quinolone (II): synthesis of fluoro-substituted pyrido[3,2-h]quinolone derivatives as potential antibacterials
AUTHOR(S): Lee, Jae Keun; Chang, Sha Joung
CORPORATE SOURCE: Dep. Chem., Coll. Natl. Sci., Taegu, 702-701, S. Korea
SOURCE: Korean Journal of Medicinal Chemistry (1994), 4(2), 92-100
PUBLISHER: KJMCE7; ISSN: 1225-0058
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



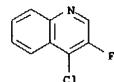
AB The potential antimicrobials, 1-ethyl-6-fluoro-1,4-dihydro-4-oxo-1,10-phenanthroline-3-carboxylic acid (I), 1-ethyl-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid and 1-ethyl-6-fluoro-1,4-dihydro-9-(4-methyl-1-piperazinyl)-4-oxo-1,10-phenanthroline-3-carboxylic acid were synthesized and their antibacterial activities were evaluated.

IT 161038-29-4P, 4-Chloro-3-fluoroquinoline

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of bactericides 4-oxo-1,10-phenanthroline-3-carboxylates)

RN 161038-28-4 CA

CN Quinoline, 4-chloro-3-fluoro- (9CI) (CA INDEX NAME)

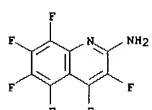


LS ANSWER 10 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 120:134243 CA
 TITLE: Remarkable orientational effects in the displacement of the fluorine from heptafluoroisoquinoline and -quinoline towards sulfur nucleophiles. Further reactions with oxygen nucleophiles
 AUTHOR(S): Brooke, Gerald M.; Chambers, Richard D.; Drury, Christopher J.; Bower, Michael J.
 CORPORATE SOURCE: Chem Dep., Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1993), (18), 2201-9
 CODEN: JCPRB4; ISSN: 0300-922X
 DOCUMENT TYPE: Journal
 LANGUAGE: English

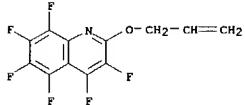
AB 1,3,4,5,6,7,8-Heptafluoroisoquinoline (I) and 2,3,4,5,6,7,8-heptafluoroquinoline (II) have been treated with a variety of sulfur and oxygen nucleophiles and some reactivities have been measured relative to treatment with ethoxide. The significant feature is that the major sites of attack by the sulfur and the oxygen nucleophiles are significantly different: attack occurs at the 6-position by sulfur and the 1-position by oxygen nucleophiles in the isoquinoline deriv. I irresp. of the relative reactivities; and at the 4-position by sulfur and at both the 2- and 4-positions by oxygen nucleophiles in the quinoline deriv. II. The results have been rationalized on the basis of the relative hardness/softness of the nucleophiles and the known activating influences of the fluorine atoms at sites remote from the reaction center.

IT 13180-57-9P
 RL: SPN (Synthetic preparation); PMP (Preparation)
 (prepn. of)

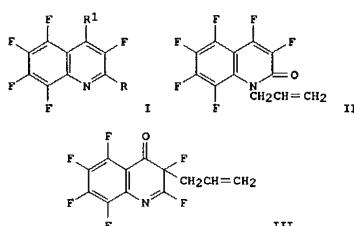
RN 13180-57-9 CA
 CN 2-Quinolinamine, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



LS ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)



LS ANSWER 11 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 110:38848 CA
 TITLE: The preparation and thermolysis reactions of allyl 3,4,5,6,7,8-hexafluoroquinolin-2-yl ether, allyl 2,3,5,6,7,8-hexafluoroquinolin-4-yl ether and allyl 3,4,5,6,7,8-hexafluoroisoquinolin-1-yl ether
 AUTHOR(S): Brooke, G. M.; Eggleston, I. M.; Hale, F. A.
 CORPORATE SOURCE: Chem. Dep., Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of Fluorine Chemistry (1988), 38(3), 421-34
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 110:38848
 GI

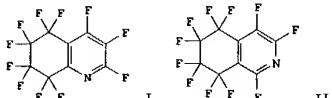


AB Reaction of CH2:CHCH2O with 2,3,4,5,6,7,8-heptafluoroquinoline gave 67 and 20% of ethers I (R = CH2:CHCH2O, R1 = F; R = F, R1 = CH2:CHCH2O), resp. Thermolysis of I (R = CH2:CHCH2O, R1 = F) in tetralin at 212.degree. for 48 h gave 69% of the Claisen rearrangement product II in which N is the migration terminus. However, a similar rearrangement of I (R = F, R1 = CH2:CHCH2O) in o-xylene at 147.5.degree. for 2.5 h gave allylquinolone III, the product with C as the migration terminus.

IT 118097-74-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PMP (Preparation); RACT (Reactant or reagent)
 (prepn. and Claisen rearrangement of)

RN 118097-74-8 CA
 CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-(2-propenyl)- (9CI) (CA INDEX NAME)

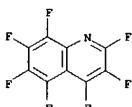
LS ANSWER 12 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 107:23214 CA
 TITLE: Polyhalogenoheterocyclic compounds. Part 37. Perfluorotetrahydroquinoline, -isoquinoline, and related compounds
 AUTHOR(S): Bell, S. L.; Chambers, R. D.; Daniels, R.; Holmes, T. F.; Silvester, M. J.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, DH1 3LE, UK
 SOURCE: Journal of Fluorine Chemistry (1986), 32(4), 403-14
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 107:23214
 GI



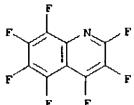
AB The formation of perfluorotetrahydroquinoline (I) and -isoquinoline II in the high temp. reaction between KF and heptachloroquinoline and -isoquinoline is investigated and a mechanism is proposed. I and II represent unusually substituted pyridine derivs. and the orientation of substitution in reactions with nucleophiles is reported.

IT 13180-38-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PMP (Preparation); RACT (Reactant or reagent)
 (prepn. and fluorination or chlorination of)

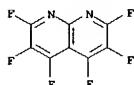
RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



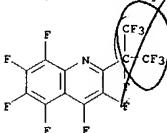
L5 ANSWER 13 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 84:135440 CA
 TITLE: Perfluorodicarboxylic acids, VI. Preparation of perfluoropyridine-2,3-dicarboxylic acid by oxidation of perfluoroquinoline
 AUTHOR(S): Sartori, P.; Ahlers, K.; Frohn, H. J.
 CORPORATE SOURCE: Fachber. Chem., Gesamthochsch. Duisburg, Duisburg, Fed. Rep. Ger.
 SOURCE: Journal of Fluorine Chemistry (1976), 7(4), 363-74
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 AB The oxidn. of perfluoroquinoline with 98% HNO₃ yields perfluoropyridine-2,3-dicarboxylic acids, 2,3,4,6,7-pentafluoro-5,8-dioxo-5,8-dihydroquinoline, and 3,4,5,6,7,8-hexafluoro-2-oxo-1,2-dihydroquinoline.
 IT 13180-38-6P
 RL: RCT (Reactant); PREP (Preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. and oxidn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



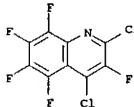
L5 ANSWER 14 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:131494 CA
 TITLE: Preparation of hexafluoro-1,8- and -2,7-naphthyridine
 AUTHOR(S): Van den Ham, D. M. W.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Journal of Fluorine Chemistry (1975), 5(6), 537-44
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Hexachloro-1,8-(I) and -2,7-naphthyridine (II) were prep'd. from 2,7-dichloro-1,8-naphthyridine and 1,3,6,8-tetrachloro-2,7-naphthyridine resp. From I and II and their starting materials a series of partially and totally fluorine substituted compds. were prep'd.
 IT 56595-12-1P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 56595-12-1 CA
 CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



L5 ANSWER 15 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 77:19504 CA
 TITLE: Reactions involving fluoride ion. V. Synthesis of perfluoro(isopropylquinolines)
 AUTHOR(S): Chambers, R. D.; Corbally, R. P.; Musgrave, W. K. R.; Jackson, J. A.; Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1286-90
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB F-induced reaction of F₃CCF₂:F₂ with perfluoroquinoline in triglyme or tetraglyme gave a mixt. of perfluoro(isopropylquinolines) (e.g. perfluoro(2,4-disopropylquinoline) (I)), substitution occurring preferentially at the 2- and 4-positions followed by attack at the 6-position. I rearranged on heating with F⁻, giving the 2,6-isomer as the main product. Unusually large coupling consts. between a 4-(CF₃)₂CF group and a 5-F atom were obsd. in the ¹⁹F NMR spectra of these compds.; the temp. dependence of the spectra was discussed in terms of preferential population of particular conformations.
 IT 36779-48-3P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 36779-48-3 CA
 CN Quinoline, 3,4,5,6,7,8-hexafluoro-2-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethyl]- (9CI) (CA INDEX NAME)



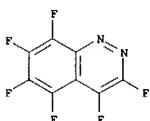
L5 ANSWER 16 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 74:53453 CA
 TITLE: Polyfluoroheterocyclic compounds. XVIII. Reactions of heptafluoroquinoline and -isquinoline and pentafluoropyridine with hydrogen halides
 AUTHOR(S): Chambers, Richard D.; Hole, M.; Musgrave, William K. R.; Thorpe, J. G.
 CORPORATE SOURCE: Sci. Lab., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1971), (1), 61-7
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB When pentafluoropyridine (I), heptafluoroquinoline (II), and heptafluoroisquinoline (III) reacted with hydrogen halides in tetrahydrothiophene dioxide, F ortho and para to ring N was replaced by the other halogen. The order of reactivity is II >> III > I. Reaction of II occurred at room temp. with substitution first at the 2- and then at the 4-position, to give 28-61% 2,4-dihalo derivs. Reaction of I or III required elevated temps.; I gave 4- and 2,4,6-substituted derivs., and III the 1-halo deriv. in low yields. Small amounts of H₂O in the solvent deactivated the system. The mechanism of the reactions is discussed in terms of nucleophilic displacement of fluoride ion from the protonated species.
 IT 27401-84-9P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 27401-84-9 CA
 CN Quinoline, 2,4-dichloro-3,5,6,7,8-pentafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 73:66535 CA
 TITLE: Hexafluorocinnoline: synthesis and photochemical isomerization to hexafluoroquinazoline
 AUTHOR(S): Chambers, Richard D.; MacBride, John A. H.; Musgrave, William K. R.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Journal of the Chemical Society [Section] D: Communications (1970), (12), 739-40
 CODEN: CCJDAO; ISSN: 0577-6171
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Hexafluorocinnoline (I) was prep'd. from hexachlorocinnoline (II) and isomerized to hexafluoroquinazoline (III) in 5-10% yields by uv irradn. at approx.100.degree.. Thus, treating IV with SO2Cl2 and Ac2O in AcOH gave V; treating V with PCl5 in POCl3 gave VI; and treating VI with Cl and AlCl3, which was fluorinated with KF to give I and 5-chloropentafluorocinnoline. I reacted rapidly with atm. moisture to give VII and with NH3 to give VIII. Volatile products from I irradn. were treated with aq. NH3 to give VIII, IX, and minor unidentified products. After irradn. of III for half the time of the I expt., 80% III was recovered with an involatile tar. I isomerization to III probably occurs via the benzodiazabenzvalene X.

IT 28734-86-3P
 RL: RCT (Reactant); PREP (Preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and photchem. rearrangement of)

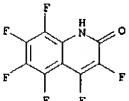
RN 28734-86-3 CA
 CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN (Continued)
 refluxed 5.5 hrs. and worked up to give 0.5 g. 2-hydroxy-4-methoxy-3,5,6,7,8-pentafluoroquinoline (VIII), m. 250-63.degree. (decompn.) (CHCl3-benzene), and 0.25 g.
 2,4-dihydroxy-3,5,6,7,8-pentafluoroquinoline (IX), m. 245-55.degree. (decompn.) (EtOAc). A mixt. of 1 g. IIIa and 1.1 g. anhyd. AlCl3 is heated 3.5 hrs. at 120.degree. and worked up to give 0.5 g. 2-hydroxy-3,4,5,6,7,8-hexafluoroquinoline (X), m. 211.degree. (decompn.) (petroleum ether-CH2Cl2); a similar demethylation of IIIb with AlCl3 gives a mixt. (m. 137.5-9.5.degree. (decompn.)) after sublimation at 80°/0.05 mm. contg. 80% 4-hydroxy-2,3,5,6,7,8-hexafluoroquinoline. To a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) is added dropwise 100 ml. H2O over 0.5 hr., and the ppt. (0.8 g.) filtered off and sublimed at 110.degree./0.1 mm. to give X. Excess CH2N2 in dry Et2O is added to a suspension of 2.35 g. X in 300 ml. dry Et2O, and the mixt. worked up to give 2.1 g. of a 9:10 mixt., sepd. by fractional sublimation and recrystn., of IV and 4-methoxy-1-methyl-3,5,6,7,8-pentafluoro-2(1H)-quinolone (XI), m. 115-16.degree.; IV and XI are also obtained in a 4:5 ratio by similarly methylating VIII, while X gives IIIa and 1-methyl-3,4,5,6,7,8-hexafluoro-2(1H)-quinolone (XII), m. 127-7.4.degree., in 2:3 ratio. A stirred mixt. of 2 g. I and 0.88 g. KOH in 50 ml. H2O is refluxed 4.25 hrs., and worked up via CH2N2 to give 1.4 g. of a mixt. of 30% IIIa, 20% IIIb and 50% XII; an analogous reaction in Me3COH gives a mixt. of 32% IIIa, 6% IIIb, and 62% XII with the same amt. of KOH, and a mixt. of 40% IIIa, 2% IIIb, 38% XII, 15% IV, and 5% XI with half again the amt. KOH. MeOH (150 ml.) is added dropwise over 1 hr. to a soln. of 1 g. I in 20 ml. H2SO4 (sp. gr. 1.84) at 0.degree., the soln. shaken with CH2Cl2, 150 ml. H2O added slowly over 1 hr., and the mixt. worked up to give 0.55 g. of a 3:17 mixt. of I and IIIa, and 0.1 g. X.

IT 13180-42-2P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 13180-42-2 CA
 CN 2(1H)-Quinolinone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



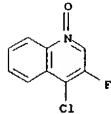
L5 ANSWER 18 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 71:81210 CA
 TITLE: Heptafluoroquinoline and derivatives
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William
 PATENT ASSIGNEE(S): K. R.
 SOURCE: National Research Development Corp.
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1155965		19690625	GB	19650513

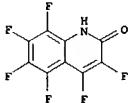
GI For diagram(s), see printed CA Issue.
 AB The title compds. are prep'd. Thus, an intimate mixt. of 31 g. heptachloroquinoline [m. 155-7.degree. (benzene), prep'd. in 78% yield from 95.5 g. tetra-chloroquinoline and 1054 g. PC15 at 315-30.degree.] and 72.5 g. anhyd. KF is heated 17 hrs. at 470.degree. in vacuo to give 18 g. of a mixt. of 85% heptafluoroquinoline (I), b. 205-5.5.degree., m. 95-5.5.degree.; 12% chloroheptafluoroquinoline isomer (II), m. 89-90.degree.; and 3% isomer of II. A soln. of 0.1 g. Na in dry MeOH is added slowly to a stirred mixt. of 1.14 g. I in 12 ml. dry MeOH, and the mixt. stirred 15 min. and worked up to give 0.91 g. of a mixt. of 97% methoxyhexafluoroquinolines (3:4:1 mixt. of IIIa-IIIb (defined below)), 28 I, and 1% 2,4-dimethoxy-3,5,6,7,8-pentafluoro-quinoline (IV), m. 107.5-8.5.degree. (MeOH), sepd. to give 2-methoxy-3,4,5,6,7,8-hexafluoroquinoline (IIIa), m. 50.5-1.5.degree., and 4-methoxy-2,3,5,6,7,8-hexafluoroquinoline (IIIb), m. 60.5-69.degree.; similar expts. with other proportions of Na give IIIa, IV, and (probably) a >9:1 mixt. of 2,4,7-and 2,4,6-trimethoxytetra-fluoroquinolines, glassy at 123-35.degree., m. 135-6.degree.. A soln. of 1.28 g. NH2H2O in 5 ml. dioxane is added over 35 min. to a stirred soln. of 30.9 g. I in 20 ml. dioxane at 20.degree., and the mixt. stirred 45 min. and worked up to give 2.95 g. solid, sublimed in vacuo to give 76% 2-hydrazino-3,4,5,6,7,8-hexafluoroquinoline (V), decompd. 196.degree. A soln. of 3.85 g. CuSO4.5H2O (VI) in 70 ml. H2O is added slowly over 45 min. to a suspension of 2.22 g. V in 50 ml. H2O, a soln. of 1.2 g. VI in 10 ml. H2O added, and the mixt. refluxed 1 hr. and worked up to give 0.5 g. solid, sublimed at 20-30.degree./0.1 mm. to give 3,4,5,6,7,8-hexafluoroquinoline, m. 62.5-4.5.degree.. Ag. NH3 (sp. gr. 0.88) (1 ml.) is added to a stirred soln. of 1 g. I in 10 ml. Me2CO at 20.degree., and the mixt. stirred 45 min. and worked up to give 0.9 g. solid, recrystd. (Me2CO-CH2Cl2) and sublimed in vacuo to give 2-amino-3,4,5,6,7,8-hexafluoroquinoline (VII), m. 224-5.degree., and a 1:4 mixt., m. 158.5-60.degree., of VII and 4-amino-2,3,5,6,7,8-hexafluoroquinoline. A mixt. of 1.25 g. IV and 15 ml. 54% eq. HI is

L5 ANSWER 19 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 70:11541 CA
 TITLE: Synthetic nucleosides and nucleotides. V. Synthesis and reaction of 3-fluoro-4-nitroquinoline 1-oxide
 AUTHOR(S): Araki, Misako; Saneyoshi, Mineo; Harada, Harue; Kawazoe, Yutaka
 CORPORATE SOURCE: Nat. Cancer Center Res. Inst., Tokyo, Japan
 SOURCE: Chemical & Pharmaceutical Bulletin (1968), 16(9), 1742-6
 CODEN: CPBTAL; ISSN: 0009-2363
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 70:11541
 GI For diagram(s), see printed CA Issue.
 AB 3-Fluoroquinoline 1-oxide, which was prep'd. through the Schiemann reaction of 3-aminoquinoline, followed by N-oxxygenation, was nitrated to 3-fluoro-4-nitroquinoline 1-oxide (I). The fluorine atom of I was replaced with nucleophiles such as OR- or NR2-contg. compds. in neutral or alk. media to afford 3-substituted 4-nitroquinoline 1-oxide derivs. The reaction with aq. HCl brought about the replacement of the nitro group to give 3-fluoro-4-chloroquinoline 1-oxide.
 IT 20849-68-7P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

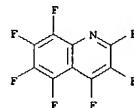
RN 20849-68-7 CA
 CN Quinoline, 4-chloro-3-fluoro-, 1-oxide (8CI) (CA INDEX NAME)



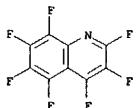
L5 ANSWER 20 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:46302 CA
 TITLE: Polyfluoroheterocyclic compounds. IX. Tautomerism
 in polyfluorohydroxyquinolines and -isoquinolines
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William
 K. R. Storey, R. A.
 CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1967), (1), 53-7
 CODEN: JSOCAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 66, 28627w. Heptafluoroquinoline with aq. NaOH or with KOH in *tert*-BuOH gives a mixt. of 2-and 4-hydroxyhexafluoroquinolines; heptafluoroisoquinoline reacts to give the 1-hydroxy deriv. 2-Hydroxyhexafluoroquinoline (I) and 1-hydroxyhexafluoroisoquinoline exist as tautomers and react with CH₂N₂ giving a mixt. of O-and N-Me derivs. whereas 4-hydroxyhexafluoroquinoline gives only an O-Me deriv. The factors affecting tautomerism in these systems are outlined.
 IT 13180-42-2P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 13180-42-2 CA
 CN 2(1H)-Quinolinone, 3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



L5 ANSWER 21 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:28627 CA
 TITLE: Polyfluoro heterocyclic compounds. VIII. Nucleophilic substitution in heptafluoroquinoline and -isoquinoline
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Musgrave, William K. R.; Storey, R. A.; Iddon, Brian
 CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (24), 2331-9
 CODEN: JSOCAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB cf. preceding abstr. Nucleophilic substitution in heptafluoroquinoline and (or) heptafluoroisoquinoline by various nucleophiles, e.g., sodium methoxide, ammonia, hydrazine, and LiAlH₄ is described. Monosubstitution and disubstitution in heptafluoroquinoline occurs at the 2-and 4-positions while in heptafluoroisoquinoline attack occurs first, specifically, at the 1-position and then at the 6-position. Oxidn. of heptafluoroisoquinoline and the methoxy derivs. gives tri- and difluoropyridinedicarboxylic acids which aid the analysis of the 19F N.M.R. spectra of the methoxy derivs. and establish their structures. Analysis of the 19F N.M.R. spectra of the derivs. of heptafluoroquinoline also clearly distinguishes their structures. In both series, some very large coupling consts. are observed which are assigned to peri F-F coupling. The major factor detg. the orientation of nucleophilic substitution in these systems is the effect of the ring nitrogen on the relative stabilities of the transition states.
 IT 13180-38-6P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



L5 ANSWER 22 OF 22 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 66:28626 CA
 TITLE: Polyfluoro heterocyclic compounds. VII. Heptafluoroquinoline and -isoquinoline
 AUTHOR(S): Chambers, Richard D.; Hole, Michael; Iddon, Brian; Musgrave, William K. R.; Storey, R. A.
 CORPORATE SOURCE: Univ. Sci. Labs., Durham, UK
 SOURCE: Journal of the Chemical Society [Section] C: Organic (1966), (24), 2328-31
 CODEN: JSOCAX; ISSN: 0022-4952
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB cf. CA 64, 7986c. Heptaachloroquinoline and -iso-quinoline have been prepd. by initial direct chlorination of quinoline and isoquinoline and subsequent reaction of the products with PO₅ at elevated temps. Reaction of these perchloro compds. with KF at elevated temps. gives heptafluoroquinoline (I) and -isoquinoline in good yields. The perchloro quinolines and isoquinolines show no basic properties except that they dissolve in concd. sulfuric acid, and that the soln. of heptafluoroquinoline on slow addn. of water or methanol gives the monohydroxy or -methoxy derivs. but on rapid diln. gives heptafluoroquinoline. The mechanism of the reaction is discussed in terms of nucleophilic displacement of fluoride ion from the protonated species.
 IT 13180-38-6P
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



10/607, 220

=> s 14 not 15
L6 18 L4 NOT L5
=> d ibib abs fhitstr hitrn 1-18

L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 140:235614 CA
 TITLE: Quinolyl propyl piperidine derivs, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
 PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
 SOURCE: Fr. Demande, 66 pp.
 CODEN: RXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MN, MX, NI, NO, NZ, OM, PG, PH, PI, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004087619	A1	20040506	US 2003-659164	20030910
PRIORITY APPLN. INFO.: FR 2002-11212			A 20020911	
OTHER SOURCE(S): MARPAT 140:235614				
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-(3-Quinol-4-yl)propylpiperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH2CO2H, CH2OH; R3 = Cl-6 alkyl substituted by: (un)substituted SPH [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2]; by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclythio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = Cl-6 alkyl, alkenyl-CH2, or alkenyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:232568 CA

TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
 PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
 SOURCE: PCT Int. Appl., 71 pp.
 CODEN: PIIXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, FR, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, NZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314
PRIORITY APPLN. INFO.: FR 2001-3374			A 20010313	
			US 2001-281407 P	20010405
			WO 2002-FR851	W 20020311
			US 2002-96482	A3 20020313
OTHER SOURCE(S): MARPAT 137:232568				
GI				

L6 ANSWER 1 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prep'd.

by N-alkylation of III (prepn. given) with 2-((2-bromoethyl)sulfonyl)-1,4-difluorobenzene, followed by acidic hydrolysis. Compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed

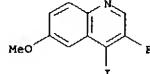
toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of quinolylpropylpiperidines as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline

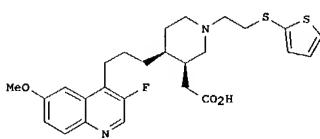
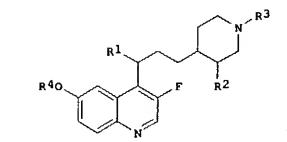
RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of quinolylpropylpiperidines as antimicrobials)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

FORMAT

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



AB New 4-(3-Quinol-4-yl)propylpiperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylaminino, dialkylaminino, hydroxylaminino, alkoxyaminino, or alkylalkoxyaminino; R2 = COOH, CH2CO2H, CH2OH; R3 = Cl-6 alkyl substituted by: (un)substituted SPH [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2]; by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclythio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms, or by (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = Cl-6 alkyl, alkenyl-CH2, or alkenyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including

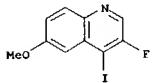
diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2H gave a 2-isomeric exocyclic olefin, which underwent hydroboration at allyl

and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II. 2HCl. Compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed

toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline

L6 ANSWER 2 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (precursor; prepn. of (quinolylpropyl)piperidine derivs. as
 antimicrobials)
 RN 426842-84-4 CA
 CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (precursor; prepn. of (quinolylpropyl)piperidine derivs. as
 antimicrobials)
 REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

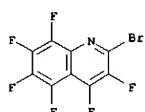
L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 13752929 CA
 TITLE: DFT Calculation of NMR JFF Spin-Spin Coupling
 Constants in Fluorinated Pyridines
 AUTHOR(S): Barone, Veronica; Peralta, Juan E.; Contreras, Ruben
 H.; Snyder, James P.
 CORPORATE SOURCE: Departamento de Fisica FCyEN, Universidad de Buenos
 Aires, Buenos Aires, Argent.
 SOURCE: Journal of Physical Chemistry A (2002), 106(23),
 5607-5612
 CODEN: JPCAFH; ISSN: 1089-5639
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB All four isotropic contributions to the NMR fluorine-fluorine coupling
 constns. (Fermi contact, FC, spin-dipolar, SD, paramagnetic spin-orbit,
 PSO, and diamagnetic spin-orbit, DSO) have been calcd. for
 2,6-difluoropyridine, 2,4,6-trifluoropyridine, perfluoropyridine, and
 2-Br-3,4,5,6,7,8-hexafluoroquinoline by means of d. functional theory in
 combination with the rather modest 6-31G** basis set. Exptl. values
 ranging from -20.3 to +45.8 Hz are semiquant. reproduced for three- to
 seven-bond couplings, suggesting that the different electronic effects
 responsible for the spin-spin interactions are adequately taken into
 account. In all cases, the relative importance of noncontact terms was
 exand. With few exceptions, the sum of the SD and PSO noncontact terms

is larger than the FC contact contribution, even though in most cases the
 two noncontact values have opposite signs. The widespread assumption that
 the

Fermi contact term dominates scalar spin-spin couplings in the case of
 light atoms would appear to be an oversimplification for JFF in
 polyfluorinated org. molis. In addn., the CPU performance of the Fermi
 contact contribution calcd. sep. by the coupled-perturbed and the
 finite-perturbation methods was investigated showing the latter to be
 slightly more efficient.

IT 60870-78-2, 2-Bromohexafluoroquinoline
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PYP (Physical process); PROC (Process)
 (DFT calcn. of NMR spin-spin coupling consts. in fluorinated
 pyridines)
 RN 60870-78-2 CA
 CN Quinoline, 2-bromo-3,4,5,6,7,8-hexafluoro- (9CI) (CA INDEX NAME)



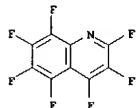
IT 60870-78-2, 2-Bromohexafluoroquinoline

L6 ANSWER 3 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 RL: PEP (Physical, engineering or chemical process); PRP (Properties);
 PYP (Physical process); PROC (Process)
 (DFT calcn. of NMR spin-spin coupling consts. in fluorinated
 pyridines)
 REFERENCE COUNT: 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR
 THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L6 ANSWER 4 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 119206380 CA
 TITLE: Extraction of perfluoroalkyl sulfonyl fluoride
 INVENTOR(S): Sato, Yukio
 PATENT ASSIGNEE(S): Tookenu Purodakutsu Kk, Japan
 SOURCE: Jpn. Kokai Tokyo Koho, 5 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168844	A2	19930702	JP 1991-65523	19910306
JP 3030661	B2	20000410		

PRIORITY APPN. INFO.: JP 1991-65523 19910306
 AB Perfluoroalkyl sulfonyl fluoride $CnF2n+1SO2F$ ($n=2-5$) in F-contg. inert
 solvents is extd. by contacting with an aq. or alc. soln. contg.
 hydroxide or carbonate of alkali or alk. earth metals, preferably selected from
 KOH, NaOH, LiOH, Ba(OH)2, K2CO3, or Li2CO3.
 IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (exth. of perfluoroalkyl sulfonic fluoride from, by potassium
 hydroxide
 soln.)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6, Perfluoroquinoline
 RL: USES (Uses)
 (exth. of perfluoroalkyl sulfonic fluoride from, by potassium
 hydroxide
 soln.)

L6 ANSWER 5 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 119:206379 CA
 TITLE: Separation of perfluoroalkyl sulfonyl fluoride
 INVENTOR(S): Sato, Yukio
 PATENT ASSIGNEE(S): Tookeno Puridakutsu Kk, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05168483	A2	19930702	JP 1991-65517	19910306
JP 3030660	B2	20000410		

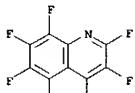
PRIORITY APPLN. INFO.: JP 1991-65517 19910306
 AB A gas contg. perfluoroalkyl sulfonic fluoride (I) $CnF2n+1SO2F$ ($n=2-5$) is contacted with a F-contg. inert solvent as an absorbent to sep. I. The gas contg. I is produced by electrolytic fluorination of alkyl sulfonic acid, alkylsulfonic fluoride, or alkylsulfonic chloride.

IT 13180-38-6, Perfluoroquinoline

RL: USES (Uses)
 (absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction
 gas mixts.)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6, Perfluoroquinoline

RL: USES (Uses)
 (absorbent, sepn. of perfluoroalkyl sulfonic fluoride by, from reaction
 gas mixts.)

L6 ANSWER 6 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 95:167967 CA
 TITLE: Proton-proton inter-ring coupling constants in isoquinoline and quinazoline. Their relationship with corresponding fluorine-19-fluorine-19 couplings in perfluoro derivatives
 AUTHOR(S): Cassidei, L.; Sciacovelli, O.
 CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70126, Italy
 SOURCE: Journal of Magnetic Resonance (1969-1992) (1981), 44(2), 340-7
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Complete spectral anal. of 1H NMR of isoquinoline and quinazoline is performed. Signs of interfering coupling consts. (JHH) are detd. by INDO expts. The mechanisms of transmission of JHH are discussed. A linear correlation exists between the majority of JHH of quinoline, isoquinoline, and quinazoline and JFF of their perfluoro derivs.; exceptions are rationalized. The linear relationship, with the near-zero value of intercept, strongly suggests that JFF originate, almost quant.,

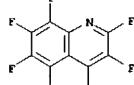
from the Fermi contact term and are transmitted via the π -electron system, except for the peri JFF . A calcn. of the proportionality between JHH and JFF in quinoline, using the Pople and Santry expression for the contribution of π -electrons to interfering coupling consts., agrees with the exptl. data.

IT 13180-38-6

RL: PRP (Properties)
 (interring proton coupling const. in quinoline vs.)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6

RL: PRP (Properties)
 (interring proton coupling const. in quinoline vs.)

L6 ANSWER 7 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 91:90752 CA
 TITLE: Relationship between proton-proton and fluorine-19-fluorine-19 inter-ring coupling constants in fused aza aromatic systems

AUTHOR(S): Cassidei, L.; Dell'Atti, A.; Sciacovelli, O.
 CORPORATE SOURCE: Ist. Chim. Fis., Univ. Bari, Bari, 70100, Italy
 SOURCE: Spectroscopy Letters (1979), 12(5), 365-9
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Inter-ring coupling consts. (JFF and JHH) in quinoline, isoquinoline, and the corresponding perfluoro derivs. were detd. The data indicate that JFF

are transmitted only through π -electrons and large stereospecific σ -img.-contributions transmitted through the all-trans pathway are absent

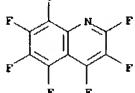
in $F-F$ coupling.

IT 13180-38-6

RL: PRP (Properties)
 (fluorine-fluorine coupling consts. in)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6

RL: PRP (Properties)
 (fluorine-fluorine coupling consts. in)

L6 ANSWER 8 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 91:67917 CA
 TITLE: Rapid general microdetermination of fluorine

AUTHOR(S): Van Leuven, H. C. E.; Rotscheid, G. J.; Buis, W. J.
 CORPORATE SOURCE: K. Shell Lab., Amsterdam, Neth.
 SOURCE: Fresenius' Zeitschrift fuer Analytische Chemie (1979), 296(1), 36-9
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB A rapid micromethod for the detn. of F in a wide variety of materials is based on the liberation of F as HF from the sample by means of pyrohydrolysis with steam at 1120. $^{\circ}$ The amt. of F in the condensate is subsequently measured with an ion-selective electrode by using simple std. addn. technique, which automatically compensates for variations in ionic strength, acidity, etc. Metals that may form stable complexes with fluoride are masked by the addn. of a complexing agent to the condensate. Materials analyzed included org. and organometallic compds., alumina-base catalysts, coal, etc. The limit of detection is of the order of 1 μ g F; the std. deviation is about 1% relative. The time

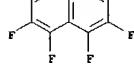
required for one detn. is 15-20 min.

IT 56595-12-1

RL: AMX (Analytical matrix); ANST (Analytical study)
 (fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)

RN 56595-12-1 CA

CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



IT 56595-12-1

RL: AMX (Analytical matrix); ANST (Analytical study)
 (fluorine detn. in, by pyrohydrolysis and subsequent potentiometry)

L6 ANSWER 9 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 87:4858 CA
 TITLE: Fluorine-19 NMR spectra of heptafluoroisoquinoline
 and

AUTHOR(S): Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Organic Magnetic Resonance (1976), 8(12), 628-31
 DOCUMENT TYPE: Journal
 LANGUAGE: English

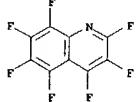
AB An anal. of the 19F NMR spectra of heptafluoroisoquinoline and hexafluoro-1-methoxyisoquinoline is presented. The inter-ring F-F coupling consts. alternate in sign and magnitude and are pos. over an odd no. of bonds. They correlated with SCF MO C-C polarizabilities inferring that the long-range coupling mechanism is dominated by the contribution from the π -electron system.

IT 13180-38-6

RL: PRP (Properties)
 (bond polarizability and π -bond order of, MO calcn. of)

RN 13180-38-6 CA

CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6

RL: PRP (Properties)
 (bond polarizability and π -bond order of, MO calcn. of)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 85:176425 CA
 TITLE: Fluorine-19 NMR spectra of polyfluoroquinolines.
 Long

AUTHOR(S): Matthews, R. S.
 CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, UK
 SOURCE: Organic Magnetic Resonance (1976), 8(5), 240-5
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The signs and magnitudes of F-F coupling consts. in perfluoroquinoline (I), 2,4-dichloropentafluoroquinoline, and 2-bromoheptafluoroquinoline were detd. by 19F NMR, providing unambiguous assignment of the spectra of I and derivs. Inter-ring F-F coupling consts. were pos. over an odd no. of bonds, and neg. over an even no. The 19F chem. shifts of I and I.F3CCO2H are reported and directly correlated with SCF MO calcd. π -electron ds. at F and bonded C atoms.

IT 60870-79-3

RL: PROC (Process)
 (fluorine-19 NMR of)

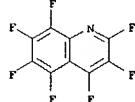
RN 60870-79-3 CA

CN Quinoline, heptafluoro-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 13180-38-6

CMF C9 F7 N



CM 2

CRN 76-05-1

CMF C2 H F3 O2



IT 60870-79-3

RL: PROC (Process)

L6 ANSWER 10 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)
 (fluorine-19 NMR of)

IT 13180-38-6 27401-84-9 60870-78-2

RL: PRP (Properties)
 (fluorine-fluorine spin coupling consts. in)

L6 ANSWER 11 OF 18 CA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 84:4155 CA
 TITLE: Electrochemical reduction of azaromatics. V.
 Influence of fluorine substitution on the electron affinities

AUTHOR(S): Van den Ham, D. M. W.; Harrison, G. F. S.; Spaans, A.;

CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1975), 94(7), 168-73
 DOCUMENT TYPE: Journal
 LANGUAGE: English

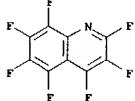
AB The electrochem. redn. process of fluoro-substituted azaromatics, e.g., 3,6-difluoropyridazine, is described by the pattern which is normally postulated for aryl halogenides, that is, fission of the C-halogen bond. However, the stability of the intermediate mononegative ions is generally higher than for the comparable fluoro-substituted arenes. As an example of this stability, the ESR spectrum of tetrafluoroquinoline is given. The half-wave redn. potentials of the first redn. wave are related to the electron affinities of the molecules. These electron affinities are correlated with those obtained by semi-empirical quantum chem. calcs.

IT 13180-38-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (electrochem. redn. of, electron affinity in relation to)

RN 13180-38-6 CA

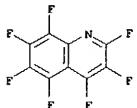
CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6

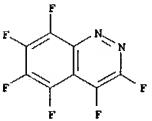
RL: RCT (Reactant); RACT (Reactant or reagent)
 (electrochem. redn. of, electron affinity in relation to)

L6 ANSWER 12 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:114335 CA
 TITLE: Reactions involving fluoride ion. XII. Reactions of polyfluoro aromatic compounds with
 octafluorobut-2-ene
 AUTHOR(S): Chambers, R. D.; Jackson, J. A.; Partington, S.;
 Philpot, P. D.; Young, A. C.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
 SOURCE: Journal of Fluorine Chemistry (1975), 6(1), 5-18
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Octafluorobut-2-ene is much more difficult to dimerize, with fluoride ion, than is hexafluoropropene but perfluoro-3,4-dimethylhex-3-ene is obtained under more forcing conditions. Polyfluoroalkylations with octafluorobut-2-ene are very efficient and results with perfluoropyridazine, -pyridine, and -pyrimidine, and quinoline are described, giving various perfluoro-2-butyl derivs. Reactions with nitropentafluorobenzene and perfluorotoluene are also described. The ¹⁹F NMR spectra of perfluoro-2-butylaromatic compds. reveal restricted rotation, even at room temp.
 IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



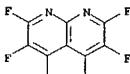
IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (perfluoroalkylation of, with octafluorobutene in presence of fluoride ion)

L6 ANSWER 14 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 80:2917 CA
 TITLE: Photoelectron spectra of some fluorine substituted diazanaphthalenes
 AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Journal of Electron Spectroscopy and Related Phenomena (1973), 2(3), 247-58
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high resolution He 584 .ANG. photoelectron spectra of unsubstituted and fluorine-substituted 1,2-, 1,3-, 1,4- and 2,3-diazanaphthalenes are presented. F substitution enables more definite anal. of the photoelectron spectra of the parent compds. Unexpected shifts of the N lone-pair bands can be explained within the through-space and through-bond interaction model and it was deduced that F substitution can give exptl. evidence about the sym. character of the lone-pair MO.
 IT 28734-86-3
 RL: PRP (Properties)
 (photoelectron spectrum of)
 RN 28734-86-3 CA
 CN Cinnoline, hexafluoro- (8CI, 9CI) (CA INDEX NAME)



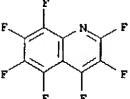
IT 28734-86-3
 RL: PRP (Properties)
 (photoelectron spectrum of)

L6 ANSWER 13 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 83:105955 CA
 TITLE: Photoelectron spectra of fluorine substituted diazanaphthalenes. Even cases
 AUTHOR(S): Van den Ham, D. M. W.; Beerlage, M.; Van der Meer, D.;
 Feil, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Journal of Electron Spectroscopy and Related Phenomena (1975), 7(1), 33-43
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high resolution He 584 .ANG. photoelectron spectra of 3 diazanaphthalenes and some of their fluoro derivs. are presented. The qualitative model that is used frequently in the discussion of lone-pair level splittings was exmd.
 IT 56595-12-1
 RL: PRP (Properties)
 (uv photoelectron spectrum and ionization potential of)
 RN 56595-12-1 CA
 CN 1,8-Naphthyridine, 2,3,4,5,6,7-hexafluoro- (9CI) (CA INDEX NAME)



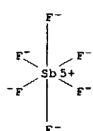
IT 56595-12-1
 RL: PRP (Properties)
 (uv photoelectron spectrum and ionization potential of)

L6 ANSWER 15 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 77:132989 CA
 TITLE: Perfluoro effect in the photoelectron spectra of quinoline and isoquinoline
 AUTHOR(S): Van den Ham, D. M. W.; Van der Meer, D.
 CORPORATE SOURCE: Chem. Phys. Lab., Twente Univ. Technol., Enschede, Neth.
 SOURCE: Chemical Physics Letters (1972), 15(4), 549-52
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The high-resoln. He 584 .ANG. photoelectron spectra of heptafluoroquinoline and heptafluoroisoquinoline are compared with those of the parent compds. Shifts in π -ionization potentials, due to the F substitution, can be described with an inductive and a combined inductive-conjugative Hueckel model.
 IT 13180-38-6
 RL: PRP (Properties)
 (photoelectron spectrum of, fluorine substitution effects in relation to)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6
 RL: PRP (Properties)
 (photoelectron spectrum of, fluorine substitution effects in relation to)

L6 ANSWER 16 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 75:117851 CA
 TITLE: Polyfluoro-heterocyclic compounds. XIX. Relative base strengths of some polyfluoroaryl-nitrogen heterocyclic systems
 AUTHOR(S): Bell, S. L.; Chambers, R. D.; Musgrave, W. K. R.; Thorpe, J. G.
 CORPORATE SOURCE: Dep. Chem., Univ. Sci. Lab., Durham, UK
 SOURCE: Journal of Fluorine Chemistry (1971), 1(1), 51-7
 CODEN: JFLCAR; ISSN: 0022-1139
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A series of hexafluoroantimonate salts of perfluoropyridine, perfluoroquinoline, perfluoroisoquinoline, and perfluoropyrazine, and of 3,5-dichlorofluoropyridine were isolated. A relative order of base strength was obtained from ^{19}F NMR measurements on mixts. of bases with acid which indicated that a dominant factor affecting base strength was the no. of F atoms ortho to the N atom.
 IT 33808-40-1
 RL: PRP (Properties)
 (basicity of, N.M.R. in relation to)
 RN 33808-40-1 CA
 CN Antimonate(1-), hexafluoro-, (OC-6-11)-, hydrogen, compd. with heptafluoroquinoline (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 16950-06-4
 CMP F6 Sb . H
 CCI CCS



● H^+

CM 2

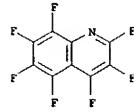
CRN 13180-38-6
 CMP C9 F7 N

L6 ANSWER 17 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 71:61301 CA
 TITLE: Acid catalyzed nucleophilic substitutions in perfluoro heterocyclic systems
 AUTHOR(S): Musgrave, William K. R.
 CORPORATE SOURCE: Univ. Durham, Durham, UK
 SOURCE: Chemistry & Industry (London, United Kingdom) (1969), (28), 943-7
 CODEN: CHINAG; ISSN: 0009-3068
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Perfluoroquinoline (I) reacted with anhyd. HCl in dried sulfolane to give 2-chlorohexafluoroquinoline, 2,4-dichloro-pentafluorquinoline, and 2-chloro-4-hydroxypentafluorquinoline. The latter was absent when sulfolane dried over mol. sieves was used. HBr gave the corresponding products only when rigorously dry sulfolane was used. Very little substitution was shown by pentafluoropyridine treated with HCl and HBr as above; however, tetrafluoropyridazine (II) was more susceptible to nucleophilic substitution, the F in positions 4 and 5 reacting 1st, while in acid soln. 3-F and 6-F were replaced 1st. When HCl was bubbled through
 II in Et2O, all 4-F atoms were replaced. AlCl_3 and AlBr_3 reacted with I at 150. $^\circ\text{C}$ to give only 2-substituted products, but AlBr_3 at >150. $^\circ\text{C}$ and AlI_3 at 150. $^\circ\text{C}$ gave 2,8-disubstituted derivs. Pentafluoropyridine decomps. when heated with Al halides; however, when the corresponding halogen acid was added, the same products were obtained as in the reactions involving the halogen acid alone.
 IT 13180-38-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, mechanism of)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6 27401-84-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (substitution reaction of, mechanism of)

L6 ANSWER 18 OF 18 CA COPYRIGHT 2004 ACS on STN (Continued)



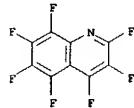
IT 33808-40-1
 RL: PRP (Properties)
 (basicity of, N.M.R. in relation to)
 IT 13180-38-6
 RL: PRP (Properties)
 (nuclear magnetic resonance of)

L6 ANSWER 18 OF 18 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 69:82102 CA
 TITLE: Ground states of conjugated molecules. X. Fluorine-19 N.M.R. chemical shifts in aryl fluorides
 AUTHOR(S): Dewar, Michael J. S.; Kelemen, Jozsef
 CORPORATE SOURCE: Univ. of Texas, Austin, TX, USA
 SOURCE: Journal of Chemical Physics (1968), 49(2), 499-508
 CODEN: JCPSA6; ISSN: 0021-9606
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The procedures developed in previous papers of this series have been extended to aromatic fluorides, by using ^{19}F N.M.R. chem. shifts as a guide to the selection of parameters for F. Attempts to correlate chem. shifts with the local π -electron d. on F proved unsatisfactory, the correlation depending on the no. of atoms ortho to F that carry p or π electrons. Similar results followed for charge d. calcd. by a recently developed semiempirical self-consistent field M.O. treatment in which all the valence electrons are included. Anal. of the Karpplus-Das-Prosser-Goodman treatment of chem. shifts suggested that this "ortho effect" arose

from neglected long-range interactions. A treatment including these was developed and shown to account well for the ^{19}F chem. shifts of nearly

100 aryl fluorides.
 IT 13180-38-6
 RL: PRP (Properties)
 (nuclear magnetic resonance of, electron configuration in relation to)
 RN 13180-38-6 CA
 CN Quinoline, heptafluoro- (8CI, 9CI) (CA INDEX NAME)



IT 13180-38-6 13323-16-5
 RL: PRP (Properties)
 (nuclear magnetic resonance of, electron configuration in relation to)

10/607,220

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FILE 'REGISTRY' ENTERED AT 15:52:20 ON 02 JUN 2004

L1 STRUCTURE UPLOADED

L2 2 S L1 SAM

L3 39 S L1 FULL

FILE 'CA' ENTERED AT 15:52:47 ON 02 JUN 2004

L4 40 S L3

L5 22 S L3/PREP

L6 18 S L4 NOT L5

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Executing the logoff script...

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STN INTERNATIONAL LOGOFF AT 15:53:57 ON 02 JUN 2004

L5 ANSWER 1 OF 5 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 140:253457 CA
 TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice
 PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.
 SOURCE: Fr. Demande, 96 pp.
 CODEN: FRXXBL
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844268	A1	20040312	FR 2002-11213	20020911
WO 2004024713	A1	20040325	WO 2003-FR2687	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004082610	A1	20040429	US 2003-659095	20030910
PRIORITY APPLN. INFO.:			FR 2002-11213	A 20020911
OTHER SOURCE(S):		MARPAT 140:253457		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1a = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R1b = H, or R1aR1b = oxo; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2 (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including various isomers, enantiomeric and diastereoisomeric forms, mixts. and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Two synthetic examples are given. For example, II was prep'd. by alkylation of III.bul.HCl (prepn. given) with

2-(bromoethylsulfanyl)thiophene, followed by basic hydrolysis. In vivo, compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c.

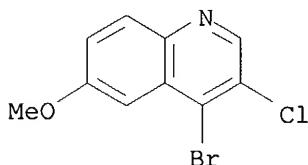
IT 426842-71-9, 4-Bromo-3-chloro-6-methoxyquinoline

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of quinolylpropyl piperidines as antimicrobial agents)

RN 426842-71-9 CA

CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CA COPYRIGHT 2004 ACS on STN

140:235614 CA

ACCESSION NUMBER:

TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials

INVENTOR(S): Bacque, Eric; Bigot, Antony; El Ahmad, Youssef; Malleron, Jean Luc; Mignani, Serge; Ronan, Baptiste; Tabart, Michel; Viviani, Fabrice

PATENT ASSIGNEE(S): Aventis Pharma SA, Fr.

SOURCE: Fr. Demande, 66 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2844270	A1	20040312	FR 2002-11212	20020911
WO 2004024712	A1	20040325	WO 2003-FR2686	20030910
W: AE, AG, AL, AU, BA, BB, BR, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RO, SC, SG, SY, TN, TT, UA, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004087619	A1	20040506	US 2003-659164	20030910
PRIORITY APPLN. INFO.:			FR 2002-11212	A 20020911
OTHER SOURCE(S):		MARPAT 140:235614		
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H or F; R2 = COOH, CH₂CO₂H, CH₂OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF₃, CF₃O, CO₂H, alkyloxycarbonyl, cyano, or NH₂], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF₃, CF₃O, oxo, COOH, alkyloxycarbonyl, cyano, or NH₂; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF₃, CF₃O, CO₂H, alkyloxycarbonyl, cyano, or NH₂], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF₃, CF₃O, oxo, COOH, alkyloxycarbonyl, cyano, or NH₂]; R4 = C1-6 alkyl, alkenyl-CH₂, or alkynyl-CH₂ (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including enantiomeric and diastereoisomeric forms, mixts. thereof, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Five synthetic examples are given. For example, II was prep'd. by N-alkylation of III (prepn. given) with 2-[(2-bromoethyl)sulfanyl]-1,4-difluorobenzene, followed by acidic hydrolysis. Compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

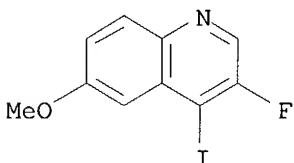
IT 426842-84-4, 4-Iodo-3-fluoro-6-methoxyquinoline

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of quinolylpropylpiperidines as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 5 CA COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 139:164798 CA

TITLE:

Preparation of aminopiperidine derivatives for treatment of bacterial infections

INVENTOR(S):

Miller, William Henry; Pearson, Neil David; Pendrak, Israil; Seefeld, Mark Andrew

PATENT ASSIGNEE(S):

Glaxo Group Limited, UK; Daines, Robert A

SOURCE:

PCT Int. Appl., 96 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003064421	A1	20030807	WO 2003-EP823	20030127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				

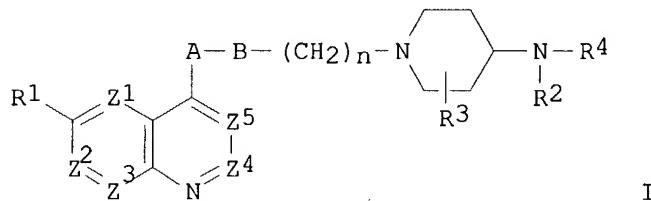
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 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
 PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
 UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
 RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
 CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
 NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW,
 ML, MR, NE, SN, TD, TG

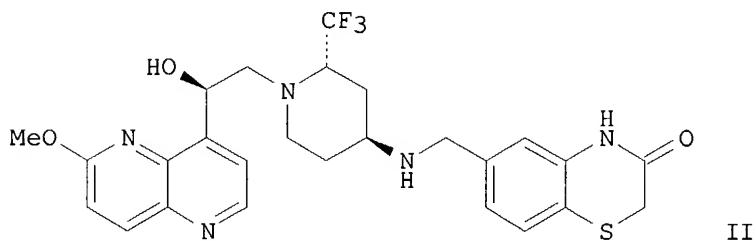
PRIORITY APPLN. INFO.: GB 2002-2026 A 20020129
 GB 2002-29824 A 20021220

OTHER SOURCE(S): MARPAT 139:164798

GI



I

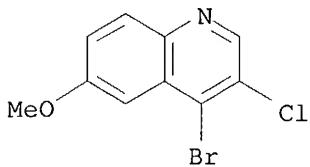


AB Title compds. I [one of Z1-5 = N, one = CR_{1a} and the remainder = CH or one of Z1-5 = CR_{1a} and the remainder = CH; R_{1-1a} = H, OH, alkoxy, amino, etc.; R₂ = H, alkyl, alkenyl; R₃ = CF₃, 2-oxo, etc.; R₄ = UR₅; U = CO, SO₂, CH₂; R₅ = bicyclic, heterocyclic ring system A; n = 0-1; AB = amido, alkylacyl, aminosulfonyl, etc.] are prep'd. For instance, bromomethyl (6-methoxy[1,5]naphthyridin-4-yl)ketone (prepn. given) is reduced (PhMe, (+)-DIPCl) to give the (R)-alc., converted to the oxirane (MeOH, K₂CO₃) and used to alkylate [(2S,4S)-2-(trifluoromethyl)piperidin-4-yl]carbamic acid tert-Bu ester (prepn. given) and deprotected to give (1R)-2-[(2S,4S)-4-amino-2-(trifluoromethyl)piperidin-1-yl]-1-(6-methoxy[1,5]naphthyridin-4-yl)ethanol. This amine is alkylated with 3-oxo-3,4-dihydro-2H-benzo[1,4]thiazine-6-carboxaldehyde (prepn. given) (EtOH, NaBH₄) to give II. Selected examples have MICs 1toreq. 2 .mu.g/mL vs., e.g., S. epidermidis CL7, S. aureus WCUH29, etc.

IT 426842-71-9P, 4-Bromo-3-chloro-6-methoxyquinoline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of aminopiperidine derivs. for treatment of bacterial

infections)
 RN 426842-71-9 CA
 CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)

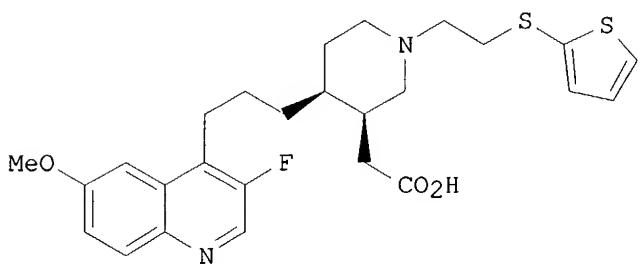
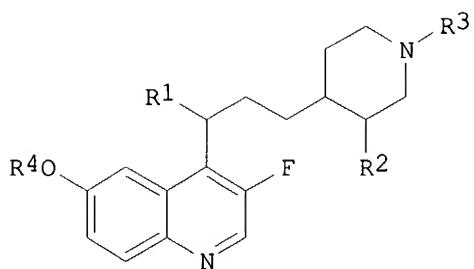


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 5 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 137:232568 CA
 TITLE: Quinolyl propyl piperidine derivatives, the preparation thereof and compositions containing same, useful as antimicrobials
 INVENTOR(S): Bacque, Eric; Mignani, Serge; Malleron, Jean-Luc; Tabart, Michel; Evers, Michel; Viviani, Fabrice; El-Ahmad, Youssef; Mutti, Stephane; Daubie, Christophe
 PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
 SOURCE: PCT Int. Appl., 71 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002072572	A1	20020919	WO 2002-FR851	20020311
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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FR 2822154	A1	20020920	FR 2001-3374	20010313
EP 1370550	A1	20031217	EP 2002-722329	20020311
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 2002177606	A1	20021128	US 2002-96482	20020313
US 6602884	B2	20030805		
US 2003171369	A1	20030911	US 2003-387479	20030314
PRIORITY APPLN. INFO.:			FR 2001-3374	A 20010313
			US 2001-281407P	P 20010405
			WO 2002-FR851	W 20020311
			US 2002-96482	A3 20020313

OTHER SOURCE(S): MARPAT 137:232568
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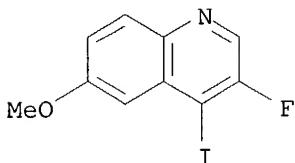


AB New 4-[3-(Quinol-4-yl)propyl]piperidine derivs. I are disclosed [wherein R1 = H, halo, OH, NH2, alkylamino, dialkylamino, hydroxyamino, alkoxyamino, or alkylalkoxyamino; R2 = COOH, CH2CO2H, CH2OH; R3 = C1-6 alkyl substituted by: (un)substituted SPh [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by 3- to 7-membered cycloalkylthio, or by 5- to 6-membered arom. heterocyclylthio comprising 1-4 N/O/S atoms and optionally substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2; or R3 = propargyl substituted by: Ph [which can include 1-4 substituents chosen from halo, OH, alkyl, alkoxy, CF3, CF3O, CO2H, alkyloxycarbonyl, cyano, or NH2], by cycloalkyl contg. 3-7 members, or by 5- to 6-membered arom. heterocyclyl with 1-4 N/O/S atoms [and (un)substituted by halo, OH, alkyl, alkoxy, CF3, CF3O, oxo, COOH, alkyloxycarbonyl, cyano, or NH2]; R4 = C1-6 alkyl, alkenyl-CH2, or alkynyl-CH2- (alkenyls or alkynyls comprise 2-6 C atoms), cycloalkyl, or cycloalkylalkyl (cycloalkyls comprises 3-8 C atoms); including diastereoisomeric forms, mixts. thereof, cis or trans forms, and salts thereof]. The novel derivs. are particularly interesting as antimicrobial agents. Ten synthetic examples are given. For instance, Wittig reaction of 4(RS)-4-allyl-1-(benzyloxycarbonyl)piperidin-3-one with Ph3P:CHCO2Me gave a Z-isomeric exocyclic olefin, which underwent hydroboration at allyl and Pd-catalyzed coupling with 4-iodo-3-fluoro-6-methoxyquinoline, followed by hydrogenation of the olefin with concomitant N-deprotection, N-alkylation with 2-(2-bromoethylthio)thiophene, and sapon. of the Me ester, to give the racemic title compd. II.2HCl. Compds. I were active against exptl. infections of mice by *Staphylococcus aureus* IP 8203 at 12-150 mg/kg s.c., and at 26-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT **426842-84-4**, 4-Iodo-3-fluoro-6-methoxyquinoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; prepn. of (quinolylpropyl)piperidine derivs. as antimicrobials)

RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



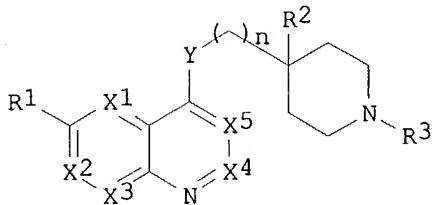
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 5 CA COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 136:386033 CA
 TITLE: Heterocyclalkyl piperidine derivatives, particularly 4-[3-(quinolin-4-yl)propyl]piperidine-4-carboxylic acids, their preparation and compositions containing same, for use as antibacterials.
 INVENTOR(S): Bacque, Eric; Carry, Jean-Christophe; El-Ahmad, Youssef; Evers, Michel; Hubert, Philippe; Malleron, Jean-Luc; Mignani, Serge; Pantel, Guy; Tabart, Michel; Viviani, Fabrice
 PATENT ASSIGNEE(S): Aventis Pharma S.A., Fr.
 SOURCE: PCT Int. Appl., 362 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

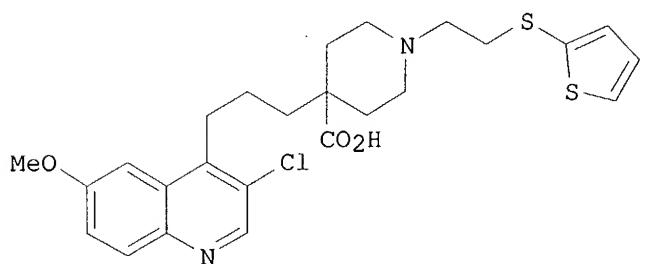
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040474	A2	20020523	WO 2001-FR3559	20011114
WO 2002040474	A3	20021031		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
FR 2816618	A1	20020517	FR 2000-14738	20001115
FR 2816618	B1	20021227		
AU 2002018365	A5	20020527	AU 2002-18365	20011114
US 2002111492	A1	20020815	US 2001-987386	20011114
US 6603005	B2	20030805		
EE 200300207	A	20030815	EE 2003-207	20011114
EP 1337529	A2	20030827	EP 2001-996538	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001015312	A	20030923	BR 2001-15312	20011114
JP 2004514661	T2	20040520	JP 2002-543484	20011114
NO 2003002187	A	20030626	NO 2003-2187	20030514
PRIORITY APPLN. INFO.:			FR 2000-14738	A 20001115
			US 2000-255145P	P 20001214
			WO 2001-FR3559	W 20011114

OTHER SOURCE(S):
GI

MARPAT 136:386033



I



II

AB The invention concerns heterocyclalkyl piperidine derivs. I, including their enantiomeric or diastereoisomeric forms, or mixts. thereof, and/or their syn or anti forms, or mixts. thereof, and their salts [wherein X1, X2, X3, X4, and X5 = C(R'1), C(R'2), C(R'3), C(R'4), C(R'5), or one of X-groups (at most) = N; R1, R'1, R'2, R'3, R'4, R'5 = H, halo, alkyl, cycloalkyl, Ph, PhS, OH, heterocyclyl, cyano, CO2H, alkoxy carbonyl, (un)substituted NH2, etc.; R2 = CO2H, alkyloxy carbonyl, cycloalkyloxy carbonyl, cyano, CONRaRb, CH2OH, substituted alkyl, CF2-Rc, C(CH3)2-Rc, CORc, CH(OH)-Rc, C(cycloalkyl)-Rc, or CH:CH-Rc; Ra, Rb = H, alkyl, cycloalkyl, Ph, heterocyclyl; or NRaRb = (un)substituted 5- or 6-membered heterocycle; Rc = CO2H, alkoxy carbonyl, cycloalkoxy carbonyl, CONRaRb; R3 = Ph, heterocyclyl, various substituted alkyls; Y = CH(Re), CF2, C(:NOH), alkyloxyiminoethylene, cycloalkyloxyiminoethylene, or C3-6 cycloalkylidene; Re = H, F, OH, alkoxy, cycloalkoxy, CO2H, alkoxy carbonyl, NRaRb, CONRaRb; and n = 0-4; wherein the radicals or Ph or heterocyclyl portions mentioned above can optionally be substituted]. Approx. 60 compds. were prep'd., 5 were specifically claimed, and many more names were listed. For instance, Pd-complex-catalyzed coupling of 4-allyl-4-Cbz-1-BOC-piperidine with 4-bromo-3-chloro-6-methoxyquinoline (preps. of both compds. given), followed by removal of the BOC group with CF3CO2H, N-alkylation with 2-[(2-bromoethyl)thio]thiophene, and hydrolysis of the benzyl ester (Cbz) in aq. HCl, gave title compd. II as the di-HCl salt. I are active against both gram-pos. and gram-neg. bacteria. I were active against exptl. infection of mice with *Staphylococcus aureus* IP8203 at 18-150 mg/kg s.c., or 20-150 mg/kg orally. None of the compds. showed toxicity in mice at 100 mg/kg s.c. (2 administrations).

IT 426842-71-9P, 4-Bromo-3-chloro-6-methoxyquinoline

426842-84-4P, 4-Iodo-3-fluoro-6-methoxyquinoline

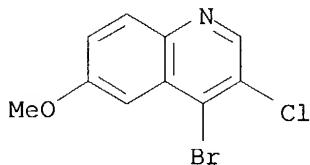
426842-86-6P, 4-Chloro-3-fluoro-6-methoxyquinoline

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of quinolinylpropylpiperidinecarboxylic acids as
antibacterials.)

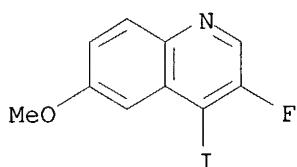
RN 426842-71-9 CA

CN Quinoline, 4-bromo-3-chloro-6-methoxy- (9CI) (CA INDEX NAME)



RN 426842-84-4 CA

CN Quinoline, 3-fluoro-4-iodo-6-methoxy- (9CI) (CA INDEX NAME)



RN 426842-86-6 CA

CN Quinoline, 4-chloro-3-fluoro-6-methoxy- (9CI) (CA INDEX NAME)

